Broadening of Andreev Bound States in $d_{x^2-y^2}$ superconductors

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We investigate the broadening of the bound states at an interface of an unconventional superconductor by bulk impurity scattering. We use the quasiclassical theory and include impurity scattering in the Born and in the unitarity limit. The broadening of bound states due to unitary scatterers is shown to be substantially weaker than in the Born limit. We study various model geometries and calculate the temperature dependence of the Josephson critical current in the presence of these impurity-broadened bound states.

I. INTRODUCTION

After a lot of discussion about the nature of the order parameter in the high-T_C materials, a number of experiments has made it virtually certain that $YBa_2Cu_3O_{7-x}$ (YBCO) is a superconductor whose order parameter has a d-wave symmetry. This was established by phase-sensitive experiments [1,2] that investigated SQUIDs or ring structures containing junctions either between YBCO and ordinary superconductors, or between different domains of YBCO.

In unconventional superconductors like those with a d-wave symmetry, the order parameter is sensitive to scattering from non-magnetic impurities and surface roughness. The order parameter also has a non-trivial structure close to surfaces and interfaces. Surfaces and interfaces can be pair-breaking, i.e., the order parameter is suppressed on a length scale given by the coherence length. Andreev reflection processes of quasi-particle excitations from the spatial profile of the order parameter, combined with conventional (and/or Andreev) reflection from the surface (interface) can result under certain conditions in surface (interface) bound states. In particular, it has been shown [3] that an interface separating two d-wave superconductors with different signs of the order parameter (in a given $\boldsymbol{k}$-direction) will *always* support a bound state at the Fermi energy. A mathematically equivalent situation arises if we consider a specularly reflecting wall and the sign of the order parameter is different for incoming and outgoing quasiparticles, i.e., there will also be a bound state.

These bound states lead to a qualitative change of the Josephson current through a tunnel junction as has been recently found in [4,5]. It was shown that the temperature dependence of the critical current is dramatically different from the standard Ambegaokar-Baratoff prediction. The critical current may increase substantially at low temperatures [4] or even change sign, i.e., the junction may change its nature from an ordinary junction to a π-junction characterized by a current-phase relation $I = I_C \sin(\phi + \pi) = -I_C \sin(\phi)$. The authors of Ref. [4] also considered the influence of surface roughness on this phenomenon and showed that it gets weaker because of a broadening of the bound states. In the present paper, we want to discuss how scattering from bulk impurities changes the bound states and, as a consequence, the Josephson critical current.

We use the quasiclassical formalism of superconductivity to obtain our results. In Section II we briefly describe the formalism. We include bulk impurities in the standard way by using an impurity self-energy. There are different models for impurity scattering, and we concentrate on two limits, viz., the limits of Born scattering (weak scattering, scattering phase shift $\delta_0 \ll 1$) and unitary scattering (strong scattering, $\delta_0 \to \pi/2$).

In Section III we calculate the angle-resolved density of states and the Josephson critical current in the presence of impurity-broadened bound states. We find by numerical calculation that bulk impurities will cut off the zero-temperature divergencies in the critical current predicted for clean systems. We also develop an analytical understanding of these results and give analytical expressions for small scattering rates. Surprisingly, we find that the bound states are more sensitive to Born scatterers than to unitary scatterers at a given scattering rate.

II. FORMALISM AND MODEL ASSUMPTIONS

In this paper, we consider the system shown in Fig. 1, consisting of a junction between two $d_{x^2-y^2}$ superconductors. The order parameter on side i, $i = L, R$ is rotated by α_i with respect to the surface normal. The junction is assumed to be weakly transparent and will be modeled as a tunnel junction. We assume that the superconductors contain a small concentration of impurities, and we would like to study the influence of these impurities on the quasiparticle bound states formed at the junction [3,4].

In unconventional superconductors, the order parameter is spatially inhomogeneous close to obstacles like surfaces or interfaces. The quasiclassical formalism of su-

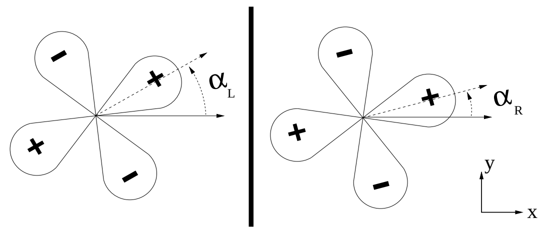

FIG. 1. Geometry of the model system: a tunnel junction between two misoriented $d_{x^2-y^2}$ superconductors

perconductivity [6–8] is ideally suited to calculating the structure of the order parameter in a self-consistent way. Its central object, the energy-integrated Green's matrix function $\hat{g}(\boldsymbol{R}, \boldsymbol{p}_{\rm F}; \varepsilon_n)$ fulfills the Eilenberger equation (we have put $\hbar = 1$)

$$[i\varepsilon_n \hat{\tau}_3 - \hat{\Delta}(\boldsymbol{R}, \boldsymbol{p}_{\rm F}) - \hat{\Sigma}(\boldsymbol{R}, \varepsilon_n), \hat{g}(\boldsymbol{p}_{\rm F}, \varepsilon_n)] + i\boldsymbol{v}_{\rm F} \boldsymbol{\nabla}_{\rm R} \hat{g}(\boldsymbol{p}_{\rm F}, \varepsilon_n) = 0 \ . \qquad (1)$$

Here $\varepsilon_n = \pi T(2n+1)$ are the Matsubara frequencies, $\hat{\Sigma}(\boldsymbol{R}, \varepsilon_n)$ is the impurity self-energy and $\hat{\tau}_i$ are the Pauli matrices.

The Green's function has to obey the normalization condition

$$\hat{g}^2(\boldsymbol{p}_{\rm F}, \varepsilon_n) = -\pi^2 \hat{1} \ , \qquad (2)$$

and $\hat{\Delta}(\boldsymbol{p}_{\rm F})$ and $\hat{g}(\boldsymbol{R}, \boldsymbol{p}_{\rm F}; \varepsilon_n)$ are related by the self-consistency relation (we have put $k_B = 1$)

$$\Delta(\boldsymbol{R}, \boldsymbol{p}_{\rm F}) = T \sum_{\varepsilon_n} \langle V(\boldsymbol{p}_{\rm F}, \boldsymbol{p}'_{\rm F}) f(\boldsymbol{R}, \boldsymbol{p}'_{\rm F}; \varepsilon_n) \rangle_{\boldsymbol{p}'_{\rm F}} \ . \qquad (3)$$

Here $\langle \ldots \rangle$ denotes averaging over the Fermi surface, which we assume to be cylindrical. The model pairing interaction is defined by

$$V(\boldsymbol{p}_{\rm F}, \boldsymbol{p}'_{\rm F}) = \lambda \cos(2\phi - 2\alpha_i) \cos(2\phi' - 2\alpha_i) \ , \qquad (4)$$

where $i = L, R$, and ϕ is the azimuthal angle between $\boldsymbol{p}_{\rm F}$ and the surface normal $\hat{\boldsymbol{n}}$.

The self-energy $\hat{\Sigma}$ describes impurity scattering, and we consider two models, viz., weak scattering (scattering phase shift $\delta_0 \ll 1$), which will be treated in the Born approximation, and unitary scattering ($\delta_0 \to \pi/2$). For an isotropic point-like impurity potential, the off-diagonal components of the self-energy vanish for order parameters transforming according to non-trivial representations of the point symmetry group of the crystal. This is the case for the d-wave order parameter studied here. The self-energy is then characterized by a single scalar function. In the Born limit the self-energy is given by

$$\Sigma(\boldsymbol{R}; \varepsilon_n) = \frac{\Gamma_b}{\pi} \langle g(\boldsymbol{R}, \boldsymbol{p}_{\rm F}; \varepsilon_n) \rangle \ , \qquad \Gamma_b = \frac{1}{2\tau} \ , \qquad (5)$$

whereas in the unitary limit

$$\Sigma(\boldsymbol{R}; \varepsilon_n) = \Gamma_u \frac{\pi}{\langle g(\boldsymbol{R}, \boldsymbol{p}_{\rm F}; \varepsilon_n) \rangle} \ , \qquad \Gamma_u = \frac{n_i}{\pi N_0} \ . \qquad (6)$$

Here, n_i is the concentration of impurities, and N_0 is the (normal) density of states at the Fermi energy.

In the framework of the quasiclassical formalism, interfaces are taken into account by Zaitsev's boundary conditions [9]. The properties of the barrier are characterized by the transmission probability $D(\boldsymbol{p}_{\rm F})$.

In the limit of zero transparency (illustrated in Fig. 2) the boundary conditions reduce to $\hat{g}(\boldsymbol{p}_{{\rm F}in}, 0+) = \hat{g}(\boldsymbol{p}_{{\rm F}out}, 0+)$. We will assume specular reflection.

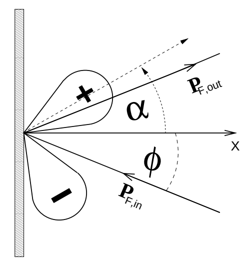

FIG. 2. Geometry of incoming and outgoing quasiparticle trajectories for an intransparent interface.

We are interested in the Josephson current through the system shown in Fig. 1. In first order in the transparency this can be expressed as

$$j_C = -\frac{eN_0^L T}{2\pi} \sum_{\varepsilon_n} \Big\langle v^L_{{\rm F}_\perp}(\boldsymbol{p}^L_{{\rm F}in}) D(\boldsymbol{p}^L_{{\rm F}in}) \big[f^L(\boldsymbol{p}^L_{{\rm F}in}; \varepsilon_n) f^{+,R}(\boldsymbol{p}^R_{{\rm F}out}; \varepsilon_n) + f^{+,L}(\boldsymbol{p}^L_{{\rm F}in}; \varepsilon_n) f^R(\boldsymbol{p}^R_{{\rm F}out}; \varepsilon_n) \big] \Big\rangle_{\boldsymbol{p}^L_{{\rm F}in}} \ , \qquad (7)$$

where the Green's functions have to be evaluated at the interface for real order parameters, as if they would not have complex phases. In the results, we will eliminate the transparency and express it through the normal-state resistance of the junction which is given by (again in first order of the transparency)

$$R_N^{-1} = e^2 A N_0^L \left\langle v^L_{{\rm F}_\perp}(\boldsymbol{p}^L_{{\rm F}in}) D(\boldsymbol{p}^L_{{\rm F}in}) \right\rangle_{\boldsymbol{p}^L_{{\rm F}in}} \ . \qquad (8)$$

In the calculation, we will assume the following model directional dependence of the transparency: $D(\phi) = D_0 \cos(\phi)^2$.

III. RESULTS FOR BORN AND UNITARY LIMIT

A surface of an unconventional superconductor may support a bound state at the Fermi energy [3,4,10]. We reproduce this phenomenon by a self-consistent solution

of a real-time version of Eqs. (1) - (3) taking into account impurity scattering. Figure 3 shows the angle-resolved local density of states (taken at the surface) obtained in the Born limit for the geometry shown in Fig. 2. The bound states present in a clean system can be seen to be broadened by impurity scattering.

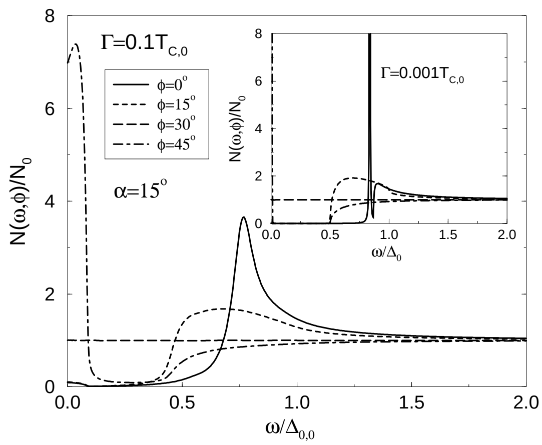

FIG. 3. Local density of states calculated for a misorientation angle of $\alpha = 15^\circ$ at a scattering rate of $\Gamma_b = 0.1 T_{C,0}$ in Born approximation. The temperature is $T = 0.01 T_{C,0}$. Inset: The same for a low scattering rate $\Gamma_b = 0.001 T_{C,0}$.

In order to estimate the dependence of the height of the zero-energy peak in the density of states on the relaxation time in the Born limit, we proceed analogously to the analytical consideration developed in [11], based on the Eilenberger equations. In particular, the residue of the Green's function for midgap states were analytically calculated there in the clean limit. Due to the presence of impurities the pole of the retarded Green's function at zero energy moves into the complex plane, although its midgap value at the surface $g(x = 0, \boldsymbol{p}_{\mathrm{F}}; \varepsilon = 0) \equiv g(\boldsymbol{p}_{\mathrm{F}}, 0)$ is still large in the case of a sufficiently large relaxation time. Under this condition we obtain the following integral equation for $g(\boldsymbol{p}_{\mathrm{F}}, 0)$:

$$
\begin{aligned}
& g(\boldsymbol{p}_{in,\mathrm{F}}, 0) \times \\
& \int\limits_0^\infty dx \left\{ \left\langle g(\boldsymbol{p'}_{\mathrm{F}}, 0) \exp\left(- \int\limits_0^x dx' \frac{2|\Delta(\boldsymbol{p'}_{\mathrm{F}}, x')|}{|v'_x|} \right) \right\rangle_{\boldsymbol{p}'_{\mathrm{F}}} \right. \\
& \times \left[\exp\left(- \int\limits_0^x dx' \frac{2|\Delta(\boldsymbol{p}_{in,\mathrm{F}}, x')|}{|v_x|} \right) + \right. \\
& \left. \left. \exp\left(- \int\limits_0^x dx' \frac{2|\Delta(\boldsymbol{p}_{out,\mathrm{F}}, x')|}{|v_x|} \right) \right] \right\} = -2\pi^2 |v_x| \tau \ . \qquad (9)
\end{aligned}
$$

The order parameter can be factorized in the form $\Delta(\boldsymbol{p}_{\mathrm{F}}, x) = \Delta_0 \psi(\boldsymbol{p}_{\mathrm{F}}, x)$. Here $\psi(\boldsymbol{p}_{\mathrm{F}}, x)$ is a dimensionless normalized function of the momentum direction and the distance from the surface ($|\psi(\boldsymbol{p}_{\mathrm{F}}, x)| \leq 1$), while Δ_0 is the maximum value of the bulk order parameter depending upon temperature and impurity concentration. The spatial dependence of $\psi(\boldsymbol{p}_{\mathrm{F}}, x)$, reduces to a dependence upon dimensionless coordinate $X = \Delta_0 x / v_F$. Introducing the dimensionless variables X, X' into Eq. (9), we see that the propagator has the form $g(\boldsymbol{p}_{\mathrm{F}}, 0) = -i\sqrt{\tau\Delta_0}\, G(\boldsymbol{p}_{\mathrm{F}}, 0)$, where $G(\boldsymbol{p}_{\mathrm{F}}, 0)$ does not contain τ and Δ_0. Hence, the height of the peak in the density of states is proportional to $\sqrt{\tau\Delta_0}$. By considering a generalization of the integral equation Eq. (9) to nonzero (although sufficiently small) values of the energy, one can show analytically that the shift of the pole position from its zero value is proportional to $\sqrt{\Delta_0/\tau}$. Thus, introducing the dimensionless quantity $\Omega_n = \varepsilon_n \sqrt{\tau/\Delta_0}$, we can represent the contribution of the midgap states to the Green's function as $g(x = 0, \boldsymbol{p}_{\mathrm{F}}; \varepsilon_n) = -i\sqrt{\tau\Delta_0}\, G(\boldsymbol{p}_{\mathrm{F}}, \Omega_n)$.

The relative strength of the influence of impurities on bound states in the Born and in the unitarity limits can be understood qualitatively by looking at Eqs. (5) and (6). In the absence of bound states, the Green's function $g(\boldsymbol{R}, \boldsymbol{p}_{\mathrm{F}}; \varepsilon_n)$ is usually quite small (compared to the normal-state value) for sufficiently small ε_n. In this case, according to Eqs. (5) and (6), the self-energy function for unitary scatterers can be significantly greater than the one in the Born limit. By contrast, if there are bound states on (or quite close to) the Fermi surface, then the corresponding large pole-like term in the expression for $g(\boldsymbol{R}, \boldsymbol{p}_{\mathrm{F}}; \varepsilon_n)$ essentially rises with decreasing temperature. This leads to the inverse situation, that is to small values of the self-energy for unitary scatterers as compared to the Born limit for the same values of the scattering rates. An analogous conclusion can be drawn for the retarded propagator and the self-energy function taken at energies close to some bound state, even if it is not at the Fermi surface. Since the pole-like term decreases with increasing Γ, the above consideration, in general, does not work for sufficiently large values of Γ_b, Γ_u. Our numerical calculations justify the above conclusion: in the presence of unitary scatterers, for sufficiently small values of Γ_u, the bound states are broadened much more weakly than in the Born limit. In contrast to the Born limit, the dependence of the propagator on the parameter Δ_0/Γ_u does not reduce to a power-law behavior in the unitarity limit, so that simple scaling estimates are not fruitful in this limit. However, some rough qualitative estimates can be done in the unitarity limit as well, in particular, by considering the simplest model d-wave order parameter, whose momentum direction dependence reduces to Δ_0 (for $0 < \phi < \pi/2$ and $\pi < \phi < 3\pi/2$) and to $-\Delta_0$ (for $\pi/2 < \phi < \pi$ and $3\pi/2 < \phi < 2\pi$). Then for small enough Γ_u we find the propagator $g(x = 0, \boldsymbol{p}_{\mathrm{F}}; \varepsilon_n = 0)$ to be proportional to $\sqrt{\Gamma_u/\Delta_0}\exp(A\Delta_0/\Gamma_u)$ with some numerical factor A of the order of unity.

We will now concentrate on the temperature and impu-

rity dependences of the Josephson critical current. Two typical and experimentally relevant geometries will be studied: the "symmetric" junction for which $\alpha_L = \alpha_R$, and the "mirror" junction for which $\alpha_L = -\alpha_R$.

In contrast to surface roughness, bulk impurities not only broaden the bound states but also change the maximum of the bulk pair potential and the critical temperature from their clean-system values $\Delta_{0,0}$ and $T_{C,0}$. This can be seen in the lower panel of Fig. 4, where the finite scattering rate leads to a renormalized value of T_C. Figure 4 shows the critical current for the symmetric geometry in Born approximation. The anomalous temperature dependence discussed in Ref. [4] is still visible, but bulk impurity cuts off the divergence at zero temperature.

We obtain an analytical estimate of the Josephson critical current in the zero-temperature limit from Eq.(7), taking into account the large low-energy values of the quantities $f^{L(R)}$, which are associated with g the same way as in the clean limit [4,11]: $f(x=0,\boldsymbol{p}_{\rm F};\varepsilon_n) = f^{+}(x=0,\boldsymbol{p}_{\rm F};\varepsilon_n) = -i\,\mathrm{sign}(v_x\Delta_\infty(\boldsymbol{p}_{\rm F}))\,g(x=0,\boldsymbol{p}_{\rm F};\varepsilon_n)$. Proceeding analogously to Ref. [4] for the symmetric (mirror) junction and introducing Ω as a new integration variable, we get

$$j_C = \pm\frac{eN_0^L}{2\pi^2}\Delta_0^{3/2}\tau^{1/2}\times \int_0^\infty d\Omega \left\langle D(\boldsymbol{p}_{\mathrm{F}in}^L) v_x^L(\boldsymbol{p}_{\mathrm{F}in}^L) G^2(X=0,\boldsymbol{p}_{\mathrm{F}in}^L,\Omega)\right\rangle_{\boldsymbol{p}_{\mathrm{F}in}^L} . \quad (10)$$

The plus (minus) sign corresponds here to the symmetric (mirror) junction.

Thus, in the Born limit and under the condition $\Delta_0\tau \gg 1$ the critical current turns out to be proportional to $\Delta_0^{3/2}\tau^{1/2}$.

In the unitarity limit, shown in Fig. 5, we find that the bound states are remarkably stable to impurity scattering, according to our conclusion made above. For sufficiently large values of Γ_u (when $\Gamma_u/T_{C,0}$ is of the order of unity), however, the influence can be substantial as can be seen in the inset to Fig. 5.

Figures 6 and 7 show the corresponding results for the mirror junction. As in Ref. [4], the critical current changes sign, i.e., the junction changes character (for some misorientation angles) and becomes a π-junction at low temperatures. Bulk impurity scattering weakens this tendency.

One simple model for a surface (or an interface) with roughness is a thin dirty layer containing Born impurities near the surface (or around the interface) [12–14,4,8]. We note that the dirty layer with unitary scatterers would influence the bound states and the Josephson critical current less strongly than in the Born limit (for the same value of the scattering rate). The problem of the most suitable model for surface and interface roughness for a given experimental situation is still open in this context.

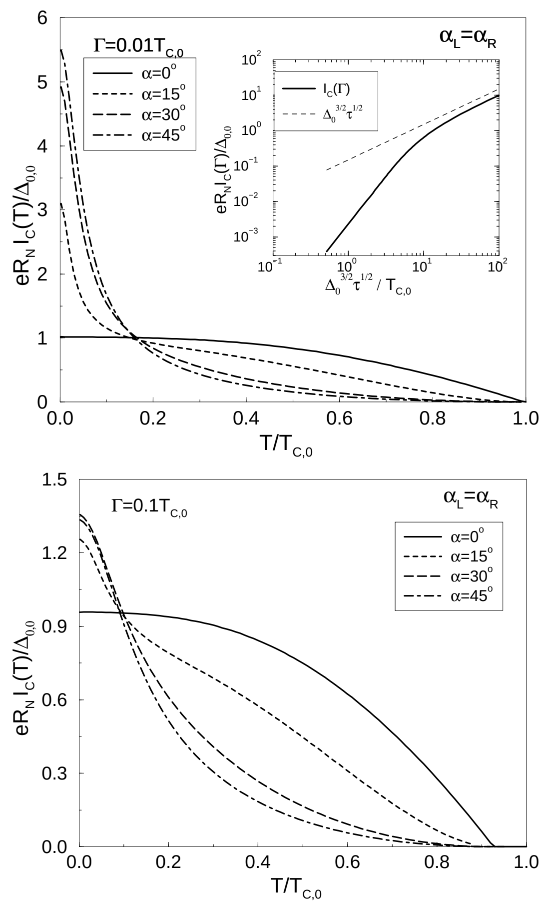

FIG. 4. Temperature dependence of the critical current for the symmetric junction, i.e., $\alpha_L = \alpha_R$ and different misorientation angles α. Impurity scattering is parameterized by the scattering rate Γ_b using the Born approximation, Eq. (5). Inset: Critical current for misorientation $\alpha = 45°$ and fixed temperature $T = 0.005T_{C,0}$ as a function of the scattering rate.

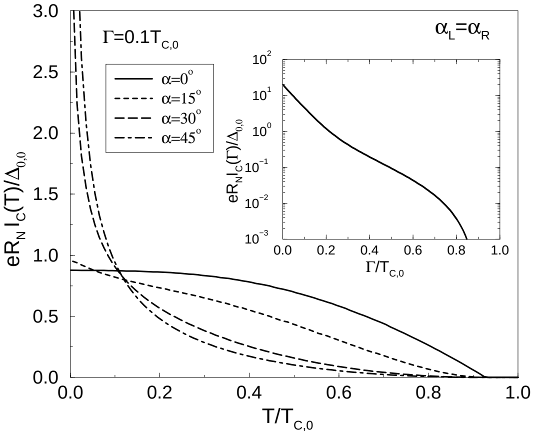

FIG. 5. Critical current as a function of temperature for the symmetric junction in the unitary limit. Inset: Critical current for misorientation $\alpha = 45^\circ$ and fixed temperature $T = 0.01T_{C,0}$ as a function of the scattering rate.

In conclusion, quasiparticle scattering by bulk impurities as well as surface roughness results in the broadening of surface (interface) quasiparticle bound states in tunnel junctions of d-wave superconductors. In this paper, we have studied this broadening due to bulk impurities and shown that scatterers can essentially reduce the height of the peak in the density of states and the low-temperature anomaly in the Josephson critical current. We have shown that bound states are more sensitive to Born scatterers than to unitary scatterers at a given value of the scattering rate. Thus, unitary scatterers would be less detrimental than Born scatterers to the observability of the low-temperature anomalies in the Josephson critical current caused by bound states.

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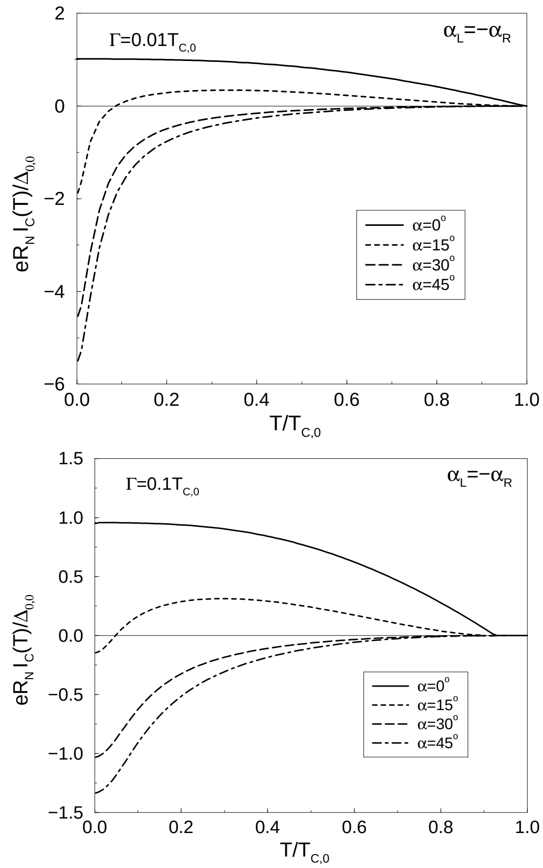

FIG. 6. Temperature dependence of the critical current for the mirror junction, i.e., $\alpha_L = -\alpha_R$ for two scattering rates Γ_b in Born approximation.

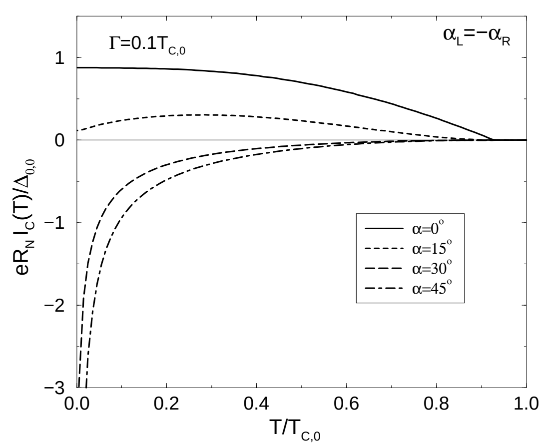

FIG. 7. Critical current as a function of temperature for the mirror junction and scattering in the unitary limit.

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